Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Quantum Monte Carlo study of charged transition-metal organometallic cluster systems[1] KAMIL TOKAR, RENE DERIAN, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences — Using accurate fixed-node quantum Monte Carlo (QMC) methods we study 1D clusters formed by transition metal atoms separated by benzene molecules (TMBz), both positively and negatively charged. TMBz are among the most important π-bonded organometallics, which, however, often require charged states for experimental studies. We have performed a systematic study of ground-sate spin multiplets, ionization potentials, electron affinities, and dissociation energies of vanadium-benzene cationic and anionic half- and full-sandwiches. By comparison of QMC and DFT results, we find a very strong impact of electronic correlation on properties of these systems, such as dissociation energies, where $\approx$1 eV energy corrections are found. In particular, the anions are unstable at the DFT level and are stabilized only at the QMC level after sophisticated optimization of the trial wavefunction.

[1]Supported by APVV-0207-11 and VEGA (2/0007/12) projects

Ivan Stich
Inst. of Physics, Slovak Academy of Sciences

Date submitted: 13 Nov 2014 Electronic form version 1.4